arXiv:0807.3999v1 [cond-mat.mes-hall] 25 Jul 2008

Properties of nano-graphite ribbons with zigzag edges – Difference between odd and even legs –

H. Yoshioka and S. Higashibata

Department of Physics, Nara Women's University, Nara 630-8506, Japan

E-mail: h-yoshi@cc.nara-wu.ac.jp

Abstract. Persistent currents and transport properties are investigated for the nano-graphite ribbons with zigzag shaped edges with paying attention to system length L dependence. It is found that both the persistent current in the isolated ring and the conductance of the system connected to the perfect leads show the remarkable L dependences. In addition, the dependences for the systems with odd legs and those with even legs are different from each other. On the persistent current, the amplitude for the cases with odd legs shows power-low behavior as L^{-N} with N being the number of legs, whereas the maximum of it decreases exponentially for the cases with even legs. The conductance per one spin normalized by e^2/h behaves as follows. In the even legs cases, it decays as L^{-2}, whereas it reaches to unity for $L \to \infty$ in the odd legs cases. Thus, the material is shown to have a remarkable property that there is the qualitative difference between the systems with odd legs and those with even legs even in the absence of the electron-electron interaction.

1. Introduction

Recently, graphite-based one-dimensional materials with nano-meter sizes have been attracting much attention in both the fundamental and applied sciences. A nano-graphite ribbon (NGR) is a nano-meter size graphite fragment and is known to have a band structure strongly depending on the shape of edges[1, 2, 3]. The NGR with zigzag shaped edges, which is schematically shown in Figure 1 and called as a zigzag NGR in the following, has a metallic band structure independent of the number of the legs N. The energy dispersion is, however, quite different from that of the regular square lattice, especially near the Fermi energy. The asymptotic behavior near the Fermi energy is given as $E(k) \sim \pm t(ka - \pi)^N$ where t is the hopping energy between the nearest neighbor atoms and a is the lattice spacing, and then the Fermi velocity vanishes. Such a singular band structure is a manifestation of the fact that the states close to the Fermi energy are localized near the zigzag edges.

In the present paper, we investigate the properties of the materials with such a remarkable band structure through the persistent current in the isolated ring pierced by the magnetic flux shown in Figure 2 and the conductance of the system attached with the perfect leads made from the regular square lattices (see Figure 3). We take care of dependences on the sample length L and on the number of the legs N. There exist already studies on the persistent current[4] and the transport properties[5, 6] of the zigzag NGR. To the best of our knowledge, however, the sample size dependences have not been discussed for the former, and the system with the present setup has not been investigated for the latter. Anomalous L dependences are found in both quantities. More interestingly, the L dependences of the even N cases and those of the odd

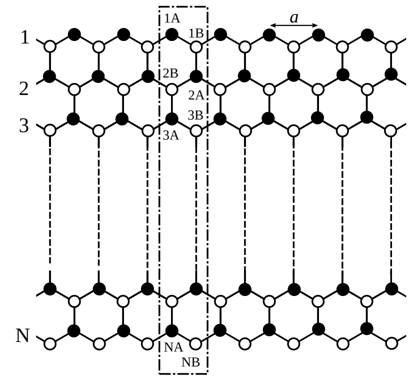

Figure 1. The structure of the zigzag NGR with N = odd. The closed (open) circles show the A (B) sublattice and the rectangle with the dash-dotted line indicates a unit cell. Here a denotes the lattice spacing.

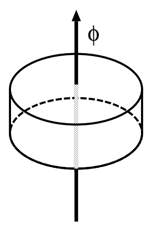

Figure 2. The ring pierced by the magnetic flux ϕ.

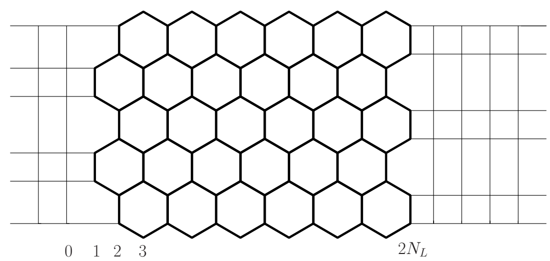

Figure 3. The zigzag NGR attached with the perfect leads, which are made from the regular square lattices.

N cases are qualitatively different from each other even in the absence of the mutual interaction.

2. Model and results

We consider the zigzag NGR consisting of N zigzag legs and the length $L = N_L a$. The spin degree of freedom is omitted because the quantities we consider are independent of the spin index and taking account of it makes these quantities twice larger. We utilize the tight-binding model with the hopping between the nearest neighbor atoms,

$$H = -t \sum_{\langle ij \rangle} \left(c_j^\dagger c_i + \mathrm{h.c.} \right), \tag{1}$$

where $\langle ij \rangle$ denotes the pair of the nearest neighbor atoms and $c_j^\dagger$ is the creation operator of the electron at the atom j. In the following, the persistent currents and the conductances are discussed based on eq. (1) in the absence of doping, in which case the Fermi level is located at the top of the valence band and at the bottom of the conduction band.

2.1. Persistent currents

The persistent current flows in the isolated rings or cylinders made from a normal metal threaded by the magnetic flux ϕ without decaying. It is a periodic function of ϕ with the period $\phi_0 = h/e$ with h and $-e$ (< 0) being the Planck constant and the electronic charge, respectively. The

current at the absolute zero temperature is obtained as follows,

$$I = -\sum_{n,k} \frac{\partial E_n(k)}{\partial \phi}, \tag{2}$$

where $E_n(k)$ is the energy dispersion with the subband n and $k = 2\pi(m + \phi/\phi_0)/L$ with m being an integer. The summations in terms of n and k are performed for $E_n(k) < 0$ because of the particle-hole symmetry of the band structure.

In the clean strict one-dimensional systems[7, 8], the persistent current behaves like a saw as a function of the magnetic flux and it's amplitude is given by ev_F/L with v_F being the Fermi velocity. In the case with finite width[8], the current also shows a saw like dependences and the maximum of the amplitude decays as L^{-1} irrespective of the number of the legs. For the zigzag NGR, the persistent current can flow in spite of the vanishing Fermi velocity[4]. Different from the square lattices, however, the current shows smooth sinusoidal dependence as a function of the flux as is shown in Figure 4 (a) and (b). We show the amplitude of the currents as a function of N_L for $N =$ odd (c) and for $N =$ even (d) in Figure 4. Obviously, the odd and even legs cases are different from each other in the L dependence. For $N_L \gg 1$, the amplitude of the former decays as N_L^{-N}, whereas the maximum values of the amplitudes for the latter show the exponential dependence. Note that we can derive the analytical expression of the amplitude for $N = 2$ as $I_{\rm amp}^{N=2} \propto \exp\left\{-N_L \ln[(9+\sqrt{17})/8]\right\}$ for $N_L \gg 1$, which reproduces the numerical result.

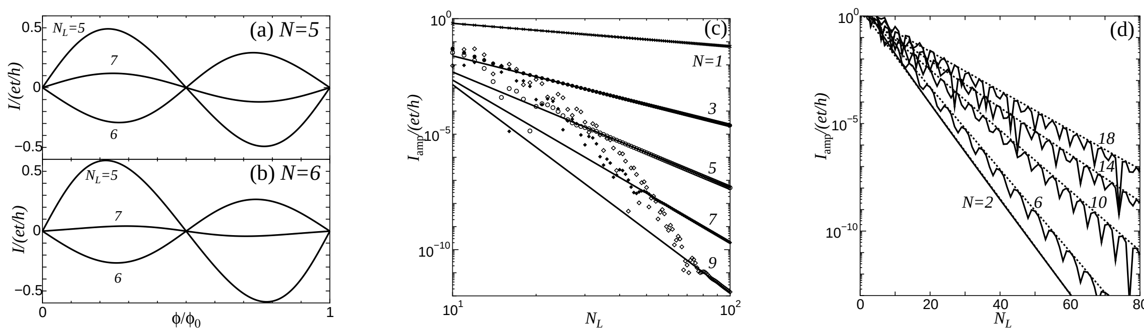

Figure 4. The persistent currents in unit of et/h as a function of the flux for $N = 5$ (a) and $N = 6$ (b). The amplitude as a function of N_L for $N =$ odd and $N =$ even are shown in (c) and (d), respectively. The solid line in each N in (c) expresses the fitting by N_L^{-N}. The dotted line in each N in (d) express the fitting of the maximum value by the exponential functions.

2.2. Conductance

According to Kohn[9], the metallic state is defined as a state with the finite Drude weight D, which can be derived in the geometry in Figure 2 as

$$D = -\lim_{L\to\infty} \pi L \left.\frac{\partial I}{\partial \phi}\right|_{\phi\to+0}, \tag{3}$$

where I is the persistent current derived in eq. (2). In this criterion, the zigzag NGR without doping is classified into an insulator due to the vanishing Fermi velocity in spite of the absence of the gap at the Fermi energy. Such an anomalous nature, therefore, is expected to lead interesting transport properties. We investigate the conductance of the system in Figure 3, where the zigzag NGR is connected to the perfect leads made from square lattices, by utilizing the recursive green

function method[10]. We note that the hopping between the nearest neighbor site in the perfect leads is assumed to be the same as that of the sample region for simplicity.

The conductance g normalized by e^2/h as a function of the sample length N_L is shown in Figure 5 for N = odd (a) and for N = even (b). As easily seen, the asymptotic behavior with

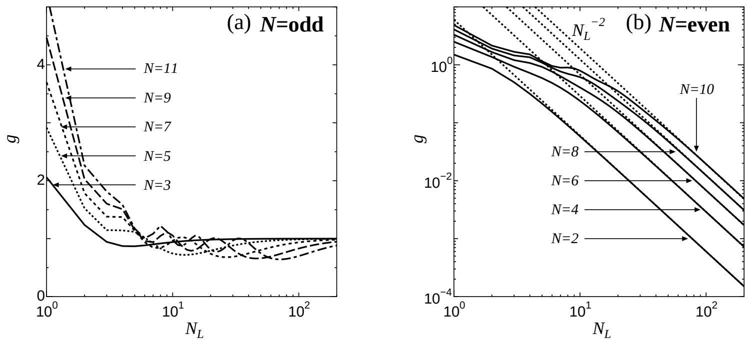

Figure 5. The conductance of the system shown in Figure 3 as a function of N_L for N = odd (a) and N = even (b).

$N_L \gg 1$ for N = odd is qualitatively different from that for N = even. In the N = odd cases, the conductance g tends to unity. On the other hand, the conductance for N = even is proportional to N_L^{-2}. Note that we can successfully obtain the analytical asymptotic ($N_L \gg 1$) expression for $N = 2$ as $g^{N=2} \simeq 6/N_L^2$, identical with the numerical result.

3. Summary and discussion

We theoretically investigated the properties of the nano-graphite ribbons with zigzag shaped edges without doping through the persistent current in the isolated ring and the conductance of the system connected to the perfect leads. Both quantities are found to show the remarkable sample length L dependence, which in the materials with even legs and with odd legs are different from each other. It seems to be very strange that qualitative differences between the N = odd and even cases appear because we cannot find clear qualitative discrepancy in the band structure. The results for N = odd seem to indicate that only the band touching the Fermi energy with the asymptotic dispersion proportional to $(ka - \pi)^N$ contributes to the both quantities as a whole. On the other hand, we suppose that strong suppressions of these quantities in N = even compared with N = odd originate from subtle cancellation. In Ref. 6, Akhmerov et al. investigated the transport properties of the zigzag NGR under the potential step and found the similar discrepancy in the conductance between the even and odd legs cases. Their model is different from ours in the origin of scattering. In the former the origin is the potential step, whereas the mismatch between the square lattice and the honeycomb lattice gives rise to the scattering in the latter. Further investigation is necessary for clarifying the mechanism leading to such strange L dependences and those differences between even and odd legs cases.

References

[1] Fujita M, Wakabayashi K, Nakada K and Kusakabe K 1996 *J. Phys. Soc. Jpn.* **65** 1920
[2] Nakada K, Fujita M, Dresselhaus G and Gresselhause M S 1996 *Phys. Rev.* B **54** 17954
[3] Wakabayashi K, Fujita M, Ajiki H and Sigrist M 1999 *Phy. Rev.* B **59** 8271
[4] Nakamura S, Wakabayashi K, Yamashiro A and Harigaya K 2004 *Physica* E **22** 684
[5] Wakabayashi K and Sigrist M 2000 *Phys. Rev. Lett.* **84** 3390
[6] Akhmerov A R, Bardarson J H, Rycerz A and Beenakker C W J 2008 *Phys. Rev.* B **77** 205416
[7] Cheung H F, Gefen Y, Riedel E K and Shi W H 1988 *Phys. Rev.* B **37** 6050
[8] Cheung H F, Gefen Y and Riedel E K 1988 *IBM J. RES. DEVELOP.* **32** 359
[9] Kohn W 1964 *Phys. Rev.* **133** A171
[10] Ando T 1991 *Phys. Rev.* B **44** 8017